Exploring Models

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INTRODUCTION

➢Major advances in environmental science require transparent, refutable models, and associated exploratory methods. Here we demonstrate a strategy introduced by Hill et al. (in review) that stresses fundamental questions addressed by a variety of methods that can be categorized as computationally frugal or demanding. Here we demonstrate the strategy using a synthetic test case with execution times long enough that computational frugality is critical to insights needed to gain transparency and refutability for this complex model.

➢Fundamental questions and associated computationally frugal and demanding methods

Model Adequacy

- **How to include many data types with variable quality?** Error-based weighting and SOO, MOO*
- **Is model misfit/overfit a problem? Are prior knowledge and data subsets inconsistent?** Variance of weight-standardized residuals, residual graphs and space/time plots, MOO*
- **How nonlinear is the problem?** Modified Beale's measure, Explore objective function*, TSDE*

Sensitivity and Uncertainty

Observations ⟷ Parameters

- **What parameters can be estimated with the observations?** b/SD_b, CSS&PCC, SV, OAT*, DoE*, FAST*, MCF(RSA)*, Sobol',* MCMC*, IR*
- **Which observations are important and unimportant to parameters?** Leverage, Cook's D, CV*, MOO*
- **Are any parameters dominated by one observation and, thus, its error?** Leverage, DFBETAS, CV*
- **How certain are the parameter values?** b/SD_b, Parameter uncertainty intervals#

Parameters ⟷ Predictions

- **Which parameters are important and unimportant to predictions?** PSS, FAST*
- **How certain are the predictions?** z/SD_z, Prediction uncertainty intervals#, MMA*
- **Which parameters contribute most and least to prediction uncertainty?** PPR, FAST*, Sobol',* MCMC*

Observations ⟷ Predictions

- **Which existing and potential observations are important to the predictions?** OPR, CV*
- **Which models in MMA are likely to produce the best predictions?** For individual model evaluations: AIC, AICc, BIC, KIC, CV*

METHODS

➢ SENSITIVITY ANALYSIS

The sensitivity analysis carried out for this work is suggested by Hill and Tiedeman (2007), and includes computationally frugal local, or gradient, methods. The relation between local and global uncertainty methods is explored by, for example. Lu et al. (2012). Local sensitivity analysis methods use the derivatives of simulated values with respect to parameters, and the derivatives are evaluated at a specific set of parameter values. Here, the sensitivity analysis uses the fit-independent composite scaled sensitivities (CSS) (defined with dimensionless scaled sensitivities DSS), parameter correlation coefficients (PCC), and leverage statistics (h), defined as:

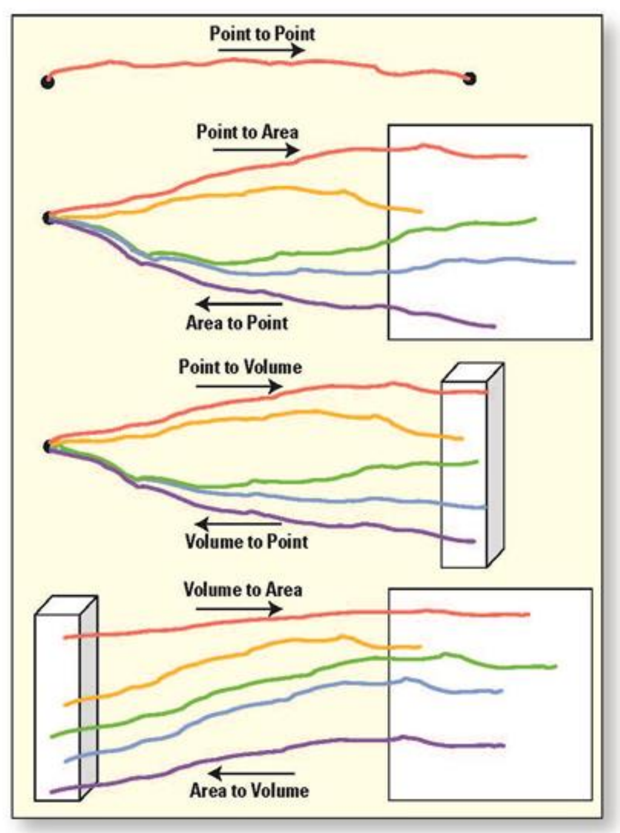
$$CSS_j = \left[\sum_{i=1}^{n} \left(DSS_{ij} \right)^2 \Big|_b / n \right]^{1/2} \qquad DSS_{ij} = \left(\partial y_i' / \partial b_j \right)_{\mathbf{b}} b_j \omega_{ii}^{1/2}$$

$$PCC_{k,\ell} = cov(b_k, b_\ell) / [var(b_k)^{1/2} \, var(b_\ell)^{1/2}] \qquad h_{ii} = \mathbf{x}_i^T \left(\mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{x}_i$$

➢ MODPATH-OBS

POINTS,AREAS, VOLUMES

Sources and sinks can be of different dimensions, as shown.



ADVECTION AND DECAY ONLY

Calculations do not include dispersion, so are most appropriate in advection dominated systems or as a first cut before more computationally intensive methods are used.

TYPES OF OBSERVATIONS SUPPORTED

- ➢ Proximity (transport reaches a given destination; useful for initial model development)
- ➢ Time of travel
- ➢ "Concentration" (use for age dating)
- ➢ Source of water

➢ MODPATH-OBOBSERVATIONS FOR TEST CASE

OBSERVATIONS

5 heads at each well and MODPATH-OBS observations as listed in the table.

ERROR-BASED OBSERVATION WEIGHTING

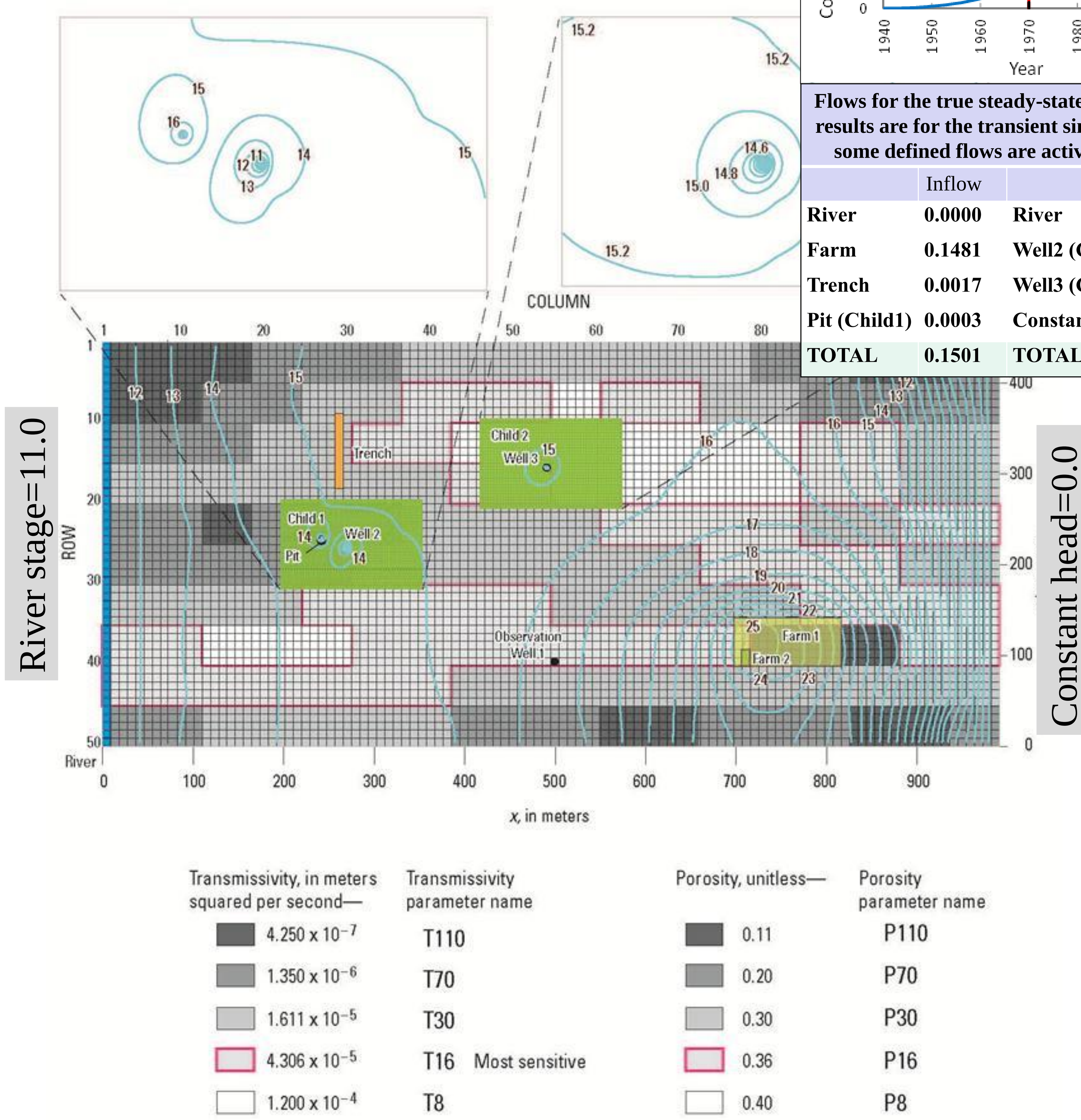
Weights are assigned based on typical errors for the types of observations supported by MODPATH-OBS, all of which are used in the test case. Weights = $1/s^2$, where s is the standard deviation.

OBS	s
Heads	0.5m
MP-OBS	Larger of 10% of obs or 1.0

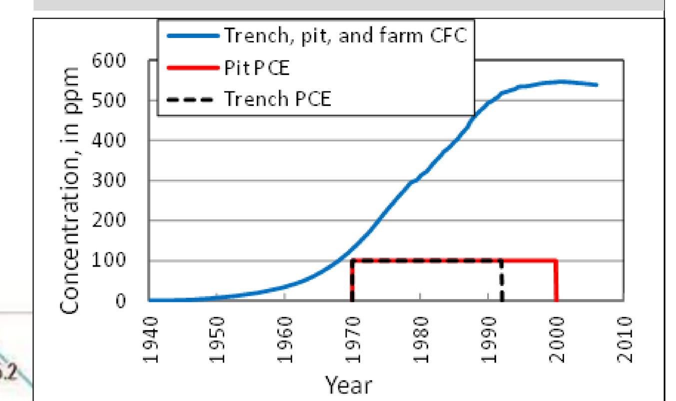
ID	Location	Source	Year	Observation	Compared
PROXIMITY, in meters from observation cell (OBSType=proximity; there are 5 observations)					
xyzobs1-3	well1	farm2	2010	0, 0, 0[5]	x, y, z-distance (Min)
xyzobs4-5	well2-3	farm2	2010	0, 0[5]	Total-distance (Min)
TIME-OF-TRAVEL, in elapsed years relative to observation (OBSType=time; there are 14 observations)					
timmedpit2	well2	pit	2010	23.38	(Med)
timmedpit2t	well2	pit	2010	1.37	(Med)—Log[7]
timminpit2 a-f	well2	pit	2005-2010	7.4 – 23.4	(Min)
timmaxpit2	well2	pit	2010	23.4	(Max)
timminall3	well3	all	2010	3.22	(Min)
timminriver3	well3	river	2010	127.68	(Min)
timminfarm3	well3	farm	2010	3.22	(Min)
timge1003	well3	all	2010	1.04	(PctGe100)
timlt1003	well3	all	2010	98.9	(PctLT100)
CONCENTRATIONS , in parts per million (OBSType=conc; there are 50 observations.)					
cnc_cfc1	well1	cfc	2010	372.5	Conc
cnc_pce1	well1	pce	2010	0. 0	Conc
cnc_cfc2a-c	well2	cfc	2008-2010	243.6 – 258.3	Conc
w2pce1970-2010	well2	pce	1970-2010	2.0 – 8.1	Conc
w2pceExc1	well2	pce	1	67.7	Exceedance (Exc1[8])
w2pceExc2	well2	pce	2	50.	Exceedance (Exc2[8])
cnc_cfc3	well3	cfc	2010	422.7	Conc
cnc_pce3	well3	pce	2010	0.57	Conc
SOURCE WATER TYPE, in percent (OBSType=source; there are 25 observations)					
typfarmto1	well1_obs	farm	2010	70.59	Percent
typ_farm2	well2_obs	farm	2000	40.4	Percent
typ_river2	well2_obs	river	2010	10.9	Percent
typ_pit3	well3_obs	pit	2010	0.0	Percent
typtrench3	well3_obs	trench	2010	0.78	Percent
typ_farm3	well3_obs	farm	2010	92.4	Percent
typ_river3	well3_obs	river	2010	0.78	Percent
tyW2Pit1970-2010	well2_obs	pit	1970-2010	0.0 – 4.7	Percent
tyW2Tr1970-2010	well2_obs	trench	1970-2010	0.0 – 5.7	Percent

SYNTHETIC APPLICATION

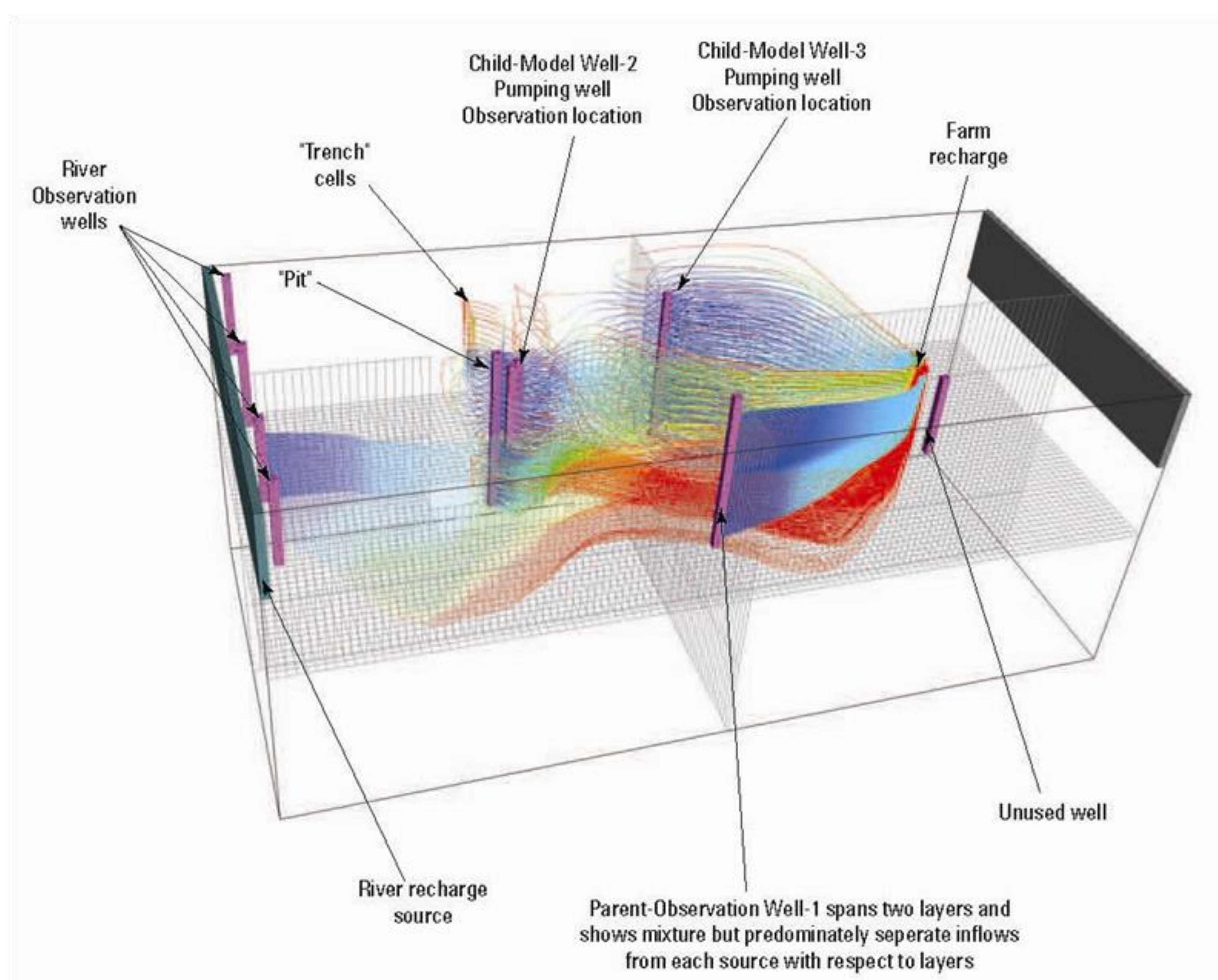
■ Area of local grid refinement to improve simulation of well hydraulics



Concentrations for defined inflow



Flows for the true steady-state simulation. Most results are for the transient simulation in which some defined flows are active limited times.			
	Inflow		Outflow
River	**0.0000**	**River**	**0.0117**
Farm	**0.1481**	**Well2 (Child1)**	**0.0022**
Trench	**0.0017**	**Well3 (Child2)**	**0.0200**
Pit (Child1)	**0.0003**	**Constant head**	**0.1161**
TOTAL	**0.1501**	**TOTAL**	**0.1500**

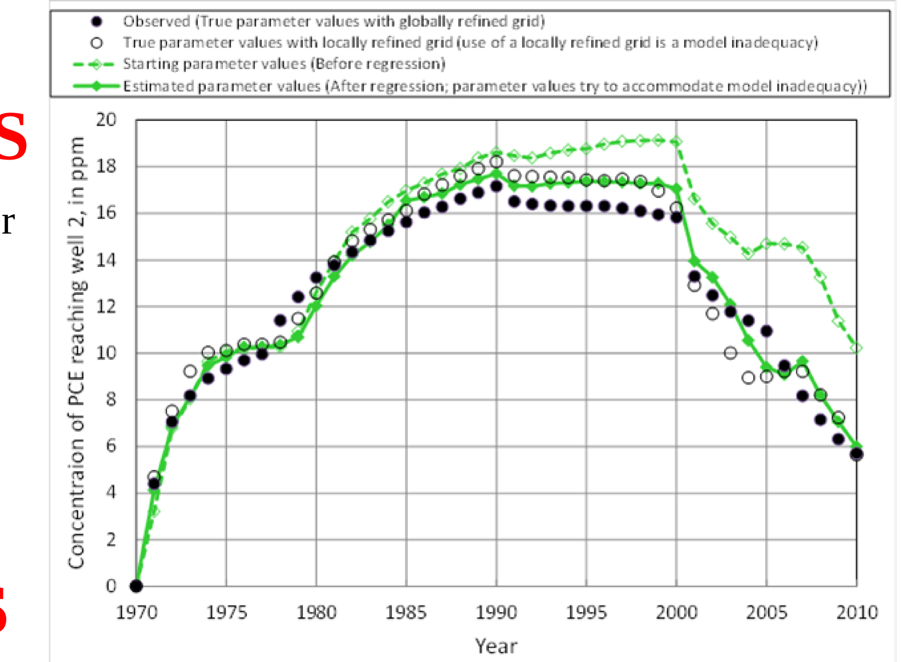


EVALUATE MODEL FIT: COMPARE SIM AND OBS

SOSWR (Sum of squared weighted residuals) for 3 parameter sets:

Start: 5606 **Estimated**: 92 **True**: 125

The figure shows concentrations over time for observation w2pce (well 2 pce concentrations). These results support the estimated parameter values and refute the starting values.

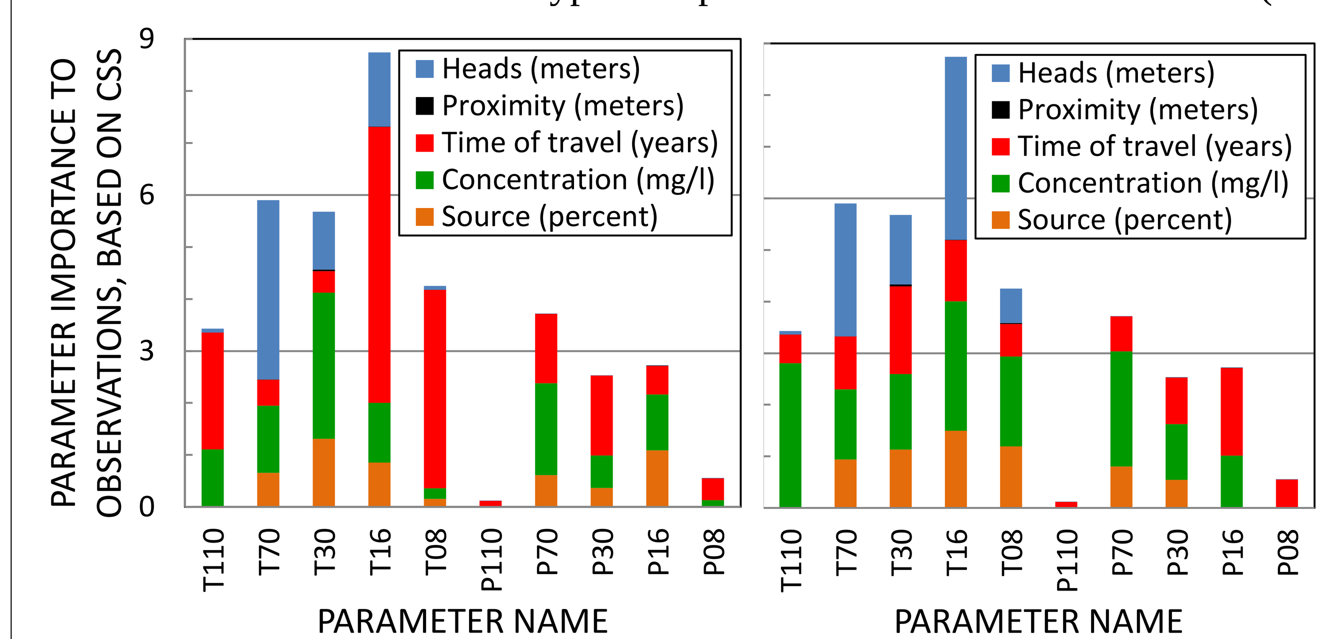


SENSITIVITY ANALYSIS

Results for 2 sets of parameter values are presented:

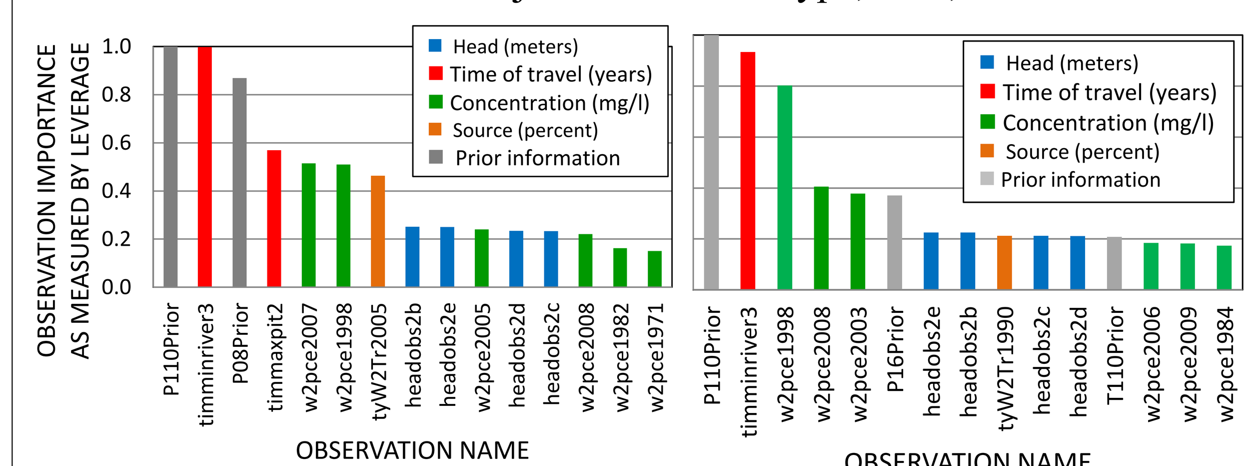
Starting (SOSWR=5606) Estimated (SOWR=92)

IMPORTANT PARAMETERS Composite scaled sensitivities (CSS) stacked by contribution from observation type and parameter correlation coefficients (PCC)..



T16 is most important; P110 is least important. Transmissivity (T) parameters tend to be more important than porosity (P) parameters. Contributing observations vary within the parameter space, but the most and least important parameters remain consistent.

IMPORTANT OBSERVATIONS Leverage identifies important observations when model fit is not considered – just observation type, time, and location. "Potentially important obs".



Leverage=1.0 means P110Prior dominates the value of at least one parameter, which clearly is parameter P110. Other top 15 observations are generally the same but the order varies with parameter value due to model nonlinearity.

Timminriver3, the time it takes the fastest particle to travel from the river to well 3, is most important.

CONCLUSIONS

The similarity in results for different parameter sets shown here and explored separately suggest the utility of local sensitivity analysis methods even for models with significant nonlinearities. The value of the kinds of insights gained in this work is highlighted by the 10,000s to 1,000,000s of model runs being conducted in many studies to obtain them.

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